

# ON THE ACCURACY OF PARTIALLY IMPLICIT SCHEMES FOR PHASE FIELD MODELING \*

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**Abstract.** Partially implicit (or partially explicit) schemes, such as the convex splitting schemes (CSS in short), are among the most popular numerical schemes used in phase-field modeling. Using both theoretical analysis and numerical experiments, we demonstrate in this paper that all existing partially implicit schemes for phase-field simulations may lack convergence accuracy. As the main example, we first show that some well-known CSS can be interpreted as some fully implicit schemes (FIS in short) in disguise. For the Allen-Cahn model, we prove that the standard CSS is exactly the same as the standard FIS but with a (much) smaller time step size and as a result, it would provide an approximation to the original solution of the Allen-Cahn model at a delayed time (although the magnitude of the delay is reduced when the time step size is reduced). Such time delay is also observed for other partially implicit schemes when time step size is not sufficient small. For the Cahn-Hilliard model, we prove that the standard CSS is exactly the same as the standard FIS for a different model that is a (nontrivial) perturbation of the original Cahn-Hilliard model. We then show that each numerical scheme on each time step can be interpreted as the discrete energy minimization problem, the convexity of which is obtained by certain restriction pertaining to the time step size. In this sense, we argue that CSS or other partially implicit scheme can be viewed as adding an artificial convexity into the discretized system.

Motivated by the equivalence between CSS and FIS, we propose a modification of a typical FIS for the Allen-Cahn model so that the maximum principle will be valid on the discrete level and we further rigorously prove that, the linearization of such a modified FIS can be uniformly preconditioned by a Poisson-like operator.

**Key words.** The Allen-Cahn model, the Cahn-Hilliard model, fully implicit schemes, convex splitting schemes.

**AMS subject classifications.** 65N12, 65N22, 65N30, 65N50.

**1. Introduction.** In this paper, we consider the following Allen-Cahn model [3]:

$$(1.1) \quad \begin{aligned} u_t - \Delta u + \frac{1}{\epsilon^2} f(u) &= 0 & \text{in } \Omega_T := \Omega \times (0, T), \\ \frac{\partial u}{\partial n} &= 0 & \text{on } \partial\Omega_T := \partial\Omega \times (0, T), \end{aligned}$$

and the following Cahn-Hilliard model [5]:

$$(1.2) \quad \begin{aligned} u_t - \Delta w &= 0 & \text{in } \Omega_T, \\ -\epsilon \Delta u + \frac{1}{\epsilon} f(u) &= w & \text{in } \Omega_T, \\ \frac{\partial u}{\partial n} = \frac{\partial w}{\partial n} &= 0 & \text{on } \partial\Omega_T. \end{aligned}$$

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The initial condition is set as  $u|_{t=0} = u_0$ . Here,  $T$  is the end time,  $\Omega \subset \mathbf{R}^d$  ( $d = 1, 2, 3$ ) is a bounded domain and  $f = F'$  for some double well potential  $F$  which, in this paper, is taken to be the following polynomial:

$$(1.3) \quad F(u) = \frac{1}{4}(u^2 - 1)^2.$$

In recent years, there have been a lot of studies in the literature on the modeling aspects and their numerical solutions for both Allen-Cahn and Cahn-Hilliard equations. For the modeling aspects, we refer to [3, 4, 5, 28, 7, 8, 14]. In this paper, we will focus on the numerical schemes for both these equations. Among the various different schemes studied in the literature, a special class of partially implicit schemes, known as convex splitting schemes (CSS), appear to be most popular, c.f. [22, 21, 19, 31, 33, 39, 17] for the Allen-Cahn equation and [22, 1, 19, 33, 31, 34, 21, 18, 15] for the Cahn-Hilliard equation. The popularity of the CSS is due to, among others, its two advantages: (1) a typical CSS is unconditionally energy-stable without any stringent restriction pertaining to the time step; (2) the resulting nonlinear numerical system can be easily solved (e.g. Newton iteration is guaranteed to converge regardless of the initial guess). In comparison, a standard fully implicit scheme is only conditionally energy-stable when the time step size is sufficiently small.

It is against our intuition and common knowledge that a convex splitting scheme, as a partially implicit scheme, has a better stability property than a fully implicit scheme. One main goal of this paper is to understand this extremely unusual phenomenon. As it turns out, in this paper, we will be able to show, rather easily, that a typical CSS is either (e.g. for Allen-Cahn) exactly equivalent to an FIS but with a much smaller time step size or (e.g. for Cahn-Hilliard) equivalent to a FIS for a regularized (and hence different) model. This at least explains theoretically why a CSS has a better stability property than a FIS does since a CSS is actually a FIS with a very small time-step size. In addition, we argue that such a gain of stability is at the expense of a possible loss of accuracy.

Given the aforementioned equivalences between CSS and FIS and the popularity of CSS in the literature, the value of FIS with a seemingly stringent time-step constraint (which, again, are equivalent to CSS without any time-step constraint) should be re-examined and that the time-step constraint imposed on the standard FIS may be acceptable. With such a motivation, in this paper, we further study two families of new algorithms for FIS. First, we propose a modification of a typical FIS for the Allen-Cahn so that the maximum principle will be valid on the discrete level. Secondly, for this modified FIS scheme, we rigorously show that, under the aforementioned appropriate time-step size constraint, the linearization of such a modified FIS can be uniformly preconditioned by a Poisson-like operator.

The second-order partially implicit schemes are designed with the same purpose of allowing large time step size as the first-order partially implicit schemes. But the serious time delay, similar to the standard CSS, happens with large time step size, which means the advantage is no longer clear for any partially implicit scheme. Actually, the second-order CSS can also be viewed as the modified Crank-Nicolson scheme [13, 33, 11] on the artificially convexified model.

The rest of paper is organized as follows. In §2, we focus on the first-order schemes. We study the convexity of the fully implicit scheme, prove that a typical CSS is exactly equivalent to some FIS. We also show that the convex splitting schemes can be viewed as artificial convexity schemes. In §3, we propose a modified FIS (or CSS) that satisfies maximum principle on the discrete level and further prove that the modified scheme can be preconditioned by a Poisson-like operator. In §4, we discuss the second-order schemes. We study a modified Crank-Nicolson scheme and its

convex splitting version, compare the modified Crank-Nicolson scheme and some other second-order partially implicit schemes. Finally, in §5, we give some concluding remarks.

**2. First-order schemes.** First, we introduce some notation. Let  $\mathcal{T}_h$  be a shape-regular (which may not be quasi-uniform) triangulation of  $\Omega \subset \mathbb{R}^d$  ( $d = 2, 3$ ). The nodes of  $\mathcal{T}_h$  is denoted by  $\mathcal{N}_h$ .  $K$  represents each element and  $\bar{\Omega} = \bigcup_{K \in \mathcal{T}_h} \bar{K}$ . Let  $h_K$  denote the diameter of  $K \in \mathcal{T}_h$  and  $h := \max\{h_K; K \in \mathcal{T}_h\}$ . Define the finite element space  $V_h$  by

$$(2.1) \quad V_h = \{v_h \in C(\bar{\Omega}) : v_h|_K = P_r(K)\},$$

where  $P_r(K)$  denotes the set of all polynomials whose degrees do not exceed a given positive integer  $r$  on  $K$ . The  $L^2$ -inner product over the domain  $\Omega$  is denoted by  $(\cdot, \cdot)$ . Given a positive integer  $N$ , let  $k := T/N$  be the time step size and  $t_n := nk$  for  $n = 0, 1, 2, \dots, N$ .

**2.1. Fully implicit schemes and their convexity and energy stability properties.** A standard fully implicit scheme to problem (1.1) (FIS in short) is defined by seeking  $u_h^n \in V_h$  for  $n = 1, 2, \dots, N$ , such that

$$(2.2) \quad \left(\frac{u_h^n - u_h^{n-1}}{k}, v_h\right) + (\nabla u_h^n, \nabla v_h) + \frac{1}{\epsilon^2}(f(u_h^n), v_h) = 0 \quad \forall v_h \in V_h.$$

A standard FIS to problem (1.2) is defined by seeking  $u_h^n \in V_h$  and  $w_h^n \in V_h$  for  $n = 1, 2, \dots, N$ , such that

$$(2.3) \quad \begin{aligned} &\left(\frac{u_h^n - u_h^{n-1}}{k}, \eta_h\right) + (\nabla w_h^n, \nabla \eta_h) = 0 \quad \forall \eta_h \in V_h, \\ &\epsilon(\nabla u_h^n, \nabla v_h) + \frac{1}{\epsilon}((u_h^n)^3 - u_h^n, v_h) - (w_h^n, v_h) = 0 \quad \forall v_h \in V_h. \end{aligned}$$

Following [14, 23], the Allen-Cahn equation (1.1) can be interpreted as the  $L^2$ -gradient flow for the free-energy functional, namely

$$(2.4) \quad \begin{aligned} J_\epsilon^{AC}(v) &:= \int_\Omega \left(\frac{1}{2}|\nabla v|^2 + \frac{1}{\epsilon^2}F(v)\right) dx, \\ \frac{d}{dt} J_\epsilon^{AC}(u(t)) &= (-\Delta u + \frac{1}{\epsilon^2}f(u), u_t)_{L^2(\Omega)} = -\|u_t\|_{L^2(\Omega)}^2 \leq 0. \end{aligned}$$

Following [2, 8, 29], the Cahn-Hilliard equation (1.2) can be interpreted as the  $H^{-1}$ -gradient flow for the free-energy functional, namely

$$(2.5) \quad \begin{aligned} J_\epsilon^{CH}(v) &:= \int_\Omega \left(\frac{\epsilon}{2}|\nabla v|^2 + \frac{1}{\epsilon}F(v)\right) dx, \\ \frac{d}{dt} J_\epsilon^{CH}(u(t)) &= (\Delta(\epsilon\Delta u - \frac{1}{\epsilon}f(u)), u_t)_{H^{-1}(\Omega)} = -\|u_t\|_{H^{-1}(\Omega)}^2 \leq 0. \end{aligned}$$

Therefore, we say that a discretization scheme such as (2.2) or (2.3) is energy-stable if

$$(2.6) \quad J_\epsilon^{AC}(u_h^n) \leq J_\epsilon^{AC}(u_h^{n-1}) \quad \text{or} \quad J_\epsilon^{CH}(u_h^n) \leq J_\epsilon^{CH}(u_h^{n-1}) \quad n = 1, 2, \dots, N.$$

We would like to point out that the concept of energy-stability for the nonlinear schemes such as (2.2) or (2.3) is different from the standard concept of stability for linear schemes. For most

linear schemes, a fully implicit scheme is usually unconditionally stable. But for nonlinear schemes, fully implicit schemes such as (2.2) or (2.3) are only conditionally energy-stable, namely they are only energy-stable when the time-step size  $k$  is appropriately small. This is well-known fact in the phase-field literature. For completeness, we will study this energy-stability property through the study of the convexity of the relevant schemes.

**2.1.1. Convexity of fully implicit schemes for the Allen-Cahn equation.** In this section, we next study the convexity property of the FIS of the Allen-Cahn and Cahn-Hilliard equations. Consider the Allen-Cahn equation, in view of (2.4), we define the following discrete energy

$$(2.7) \quad E(u, u_h^{n-1}) = J_\epsilon^{AC}(u) + \frac{1}{2k} \int_\Omega (u - u_h^{n-1})^2 dx.$$

**THEOREM 2.1.** *Under the condition that  $k \leq \epsilon^2$ , we have*

1.  $E(\cdot, u_h^{n-1})$  is strictly convex on  $H^1(\Omega)$ .
2. The equation (2.2) satisfies  $u_h^n = \underset{v_h \in V_h}{\operatorname{argmin}} E(v_h, u_h^{n-1})$ .
3. The following discrete energy law holds

$$(2.8) \quad J_\epsilon^{AC}(u_h^n) + \frac{1}{2k} \|u_h^n - u_h^{n-1}\|_{L^2(\Omega)}^2 \leq J_\epsilon^{AC}(u_h^{n-1}).$$

*Proof.* Taking the second derivative of  $E(\cdot, u_h^{n-1})$ , we get

$$(2.9) \quad E''(u, u_h^{n-1})(v, v) = \frac{3}{\epsilon^2} \int_\Omega u^2 v^2 dx + \int_\Omega \left(\frac{1}{k} - \frac{1}{\epsilon^2}\right) v^2 dx + \|\nabla v\|_{L^2(\Omega)}^2.$$

When  $k \leq \epsilon^2$ ,  $E''(u, u_h^{n-1})(v, v) > 0$  when  $v \neq 0$ , which means  $E(\cdot, u_h^{n-1})$  is strictly convex. Notice that (2.2) implies that  $E'(u_h^n, u_h^{n-1})(v_h) = 0$ , and the following coercivity condition holds:

$$(2.10) \quad E(u_h, u_h^{n-1}) \geq M_1 \|u_h\|_{H^1(\Omega)}^2 - M_2,$$

where  $M_1$  and  $M_2$  are positive constants that depend on  $\epsilon$ . Then the unique solvability of the minimizer  $u_h^n$  follows from [10] and (2.10). Moreover, we have

$$J_\epsilon^{AC}(u_h^n) + \frac{1}{2k} \|u_h^n - u_h^{n-1}\|_{L^2(\Omega)}^2 = E(u_h^n, u_h^{n-1}) \leq E(u_h^{n-1}, u_h^{n-1}) = J_\epsilon^{AC}(u_h^{n-1}).$$

Then we finish the proof.  $\square$

In view of Theorem 2.1, let us introduce the terminology of *convex scheme*. We say that a scheme is *convex* if it is equivalent to the minimization of a convex functional. Thus (2.2) is a convex scheme under the condition  $k \leq \epsilon^2$ . Theorem 2.1 also shows the energy stability of (2.2) follows from its convexity.

**2.1.2. Convexity of fully implicit scheme for the Cahn-Hilliard equation.** Define the discrete Laplace operator  $\Delta_h : V_h \mapsto V_h$  as follows: Given  $v_h \in V_h$ , let  $\Delta_h v_h \in V_h$  such that

$$(2.11) \quad (\Delta_h v_h, w_h) = -(\nabla v_h, \nabla w_h) \quad \forall w_h \in V_h.$$

Let  $L_0^2$  denote the collection of functions in  $L^2(\Omega)$  with zero mean, and let  $\mathring{V}_h := V_h \cap L_0^2$ . Taking  $w_h = 1$  in (2.11), we know that  $\operatorname{Range}(\Delta_h) \subset \mathring{V}_h$ . Further, the well-posedness of the Poisson

problem with Neumann boundary condition on  $\mathring{V}_h$  implies that  $\text{Range}(\Delta_h) = \mathring{V}_h$ . Therefore,  $\Delta_h|_{\mathring{V}_h} : \mathring{V}_h \mapsto \mathring{V}_h$  is an isomorphism, then  $\Delta_h^{-1} := (\Delta_h|_{\mathring{V}_h})^{-1} : \mathring{V}_h \mapsto \mathring{V}_h$  is well-defined.

Consider the Cahn-Hilliard equations, in view of (2.5), we define the discrete energy

$$(2.12) \quad \hat{E}(\theta_h, u_h^{n-1}) = J_\epsilon^{CH}(u_h^{n-1} + \theta_h) + \frac{1}{2k} \|\nabla \Delta_h^{-1} \theta_h\|_{L^2(\Omega)}^2 \quad \theta_h \in \mathring{V}_h.$$

**THEOREM 2.2.** *Under the condition that  $k \leq 4\epsilon^3$ , we have*

1.  $\hat{E}(\cdot, u_h^{n-1})$  is convex on  $\mathring{V}_h$ .
2. The solution of (2.3) satisfies  $u_h^n = u_h^{n-1} + \theta_h$ , with  $\theta_h = \underset{\eta_h \in \mathring{V}_h}{\operatorname{argmin}} \hat{E}(\eta_h, u_h^{n-1})$ .
3. The following energy law holds

$$(2.13) \quad J_\epsilon^{CH}(u_h^n) + \frac{1}{2k} \|\nabla \Delta_h^{-1}(u_h^n - u_h^{n-1})\|_{L^2(\Omega)}^2 \leq J_\epsilon^{CH}(u_h^{n-1}).$$

*Proof.* For any  $\theta_h, \eta_h \in \mathring{V}_h$ , we have

$$\hat{E}''(\theta_h, u_h^{n-1})(\eta_h, \eta_h) = \frac{1}{\epsilon} \int_\Omega (3(u_h^{n-1} + \theta_h)^2 - 1) \eta_h^2 dx + \frac{1}{k} \|\nabla \Delta_h^{-1} \eta_h\|_{L^2(\Omega)}^2 + \epsilon \|\nabla \eta_h\|_{L^2(\Omega)}^2.$$

Using Schwarz's inequality, we have

$$\frac{1}{\epsilon} \|\eta_h\|_{L^2(\Omega)}^2 \leq \frac{1}{\epsilon} (\Delta_h^{-1} \eta_h, \eta_h)^{1/2} (\Delta_h \eta_h, \eta_h)^{1/2} \leq \frac{1}{4\epsilon^3} \|\nabla \Delta_h^{-1} \eta_h\|_{L^2(\Omega)}^2 + \epsilon \|\nabla \eta_h\|_{L^2(\Omega)}^2.$$

When  $k \leq 4\epsilon^3$ ,

$$(2.14) \quad \hat{E}''(\theta_h, u_h^{n-1})(\eta_h, \eta_h) \geq \frac{1}{\epsilon} \int_\Omega 3(u_h^{n-1} + \theta_h)^2 \eta_h^2 dx + \left(\frac{1}{k} - \frac{1}{4\epsilon^3}\right) \|\nabla \Delta_h^{-1} \eta_h\|_{L^2(\Omega)}^2 \geq 0,$$

where the strict inequality holds when  $\eta_h \neq 0$ . This means that  $\hat{E}(\cdot, u_h^{n-1})$  is strictly convex on  $\mathring{V}_h$ .

Now, taking  $\eta_h = 1$  in (2.3), we have  $u_h^n \in u_h^{n-1} + \mathring{V}_h$ . Let  $v_h = 1$  in (2.3), we have  $\int_\Omega w_h^n dx = \frac{1}{\epsilon} \int_\Omega f(u_h^n) dx$ . Then, the first equation of (2.3) is equivalent to

$$w_h^n = \frac{1}{k} \Delta_h^{-1}(u_h^n - u_h^{n-1}) + \frac{1}{\epsilon|\Omega|} \int_\Omega f(u_h^n) dx.$$

Therefore, (2.3) is shown to be

$$(2.15) \quad \epsilon(\nabla u_h^n, \nabla v_h) + \frac{1}{\epsilon} ((I - Q_0)f(u_h^n), v_h) - \frac{1}{k} (\Delta_h^{-1}(u_h^n - u_h^{n-1}), v_h) = 0 \quad \forall v_h \in V_h.$$

where  $Q_0 : L^2(\Omega) \mapsto \mathbb{R}$  is the  $L^2$  projection, namely  $Q_0 v = \frac{1}{|\Omega|} \int_\Omega v dx$ . Let  $\theta_h = u_h^n - u_h^{n-1} \in \mathring{V}_h$ . Note that  $Q_0 \theta_h = Q_0 \Delta^{-1} \theta_h = 0$ , we can then write (2.15) as

$$\epsilon(\nabla(u_h^{n-1} + \theta_h), \nabla(I - Q_0)v_h) + \frac{1}{\epsilon} (f(u_h^{n-1} + \theta_h), (I - Q_0)v_h) - \frac{1}{k} (\Delta_h^{-1} \theta_h, (I - Q_0)v_h) = 0 \quad \forall v_h \in V_h.$$

This means that

$$\epsilon(\nabla(u_h^{n-1} + \theta_h), \nabla v_h) + \frac{1}{\epsilon} (f(u_h^{n-1} + \theta_h), v_h) - \frac{1}{k} (\Delta_h^{-1} \theta_h, v_h) = 0 \quad \forall v_h \in \mathring{V}_h,$$

which is equivalent to the minimization problem  $\theta_h = \underset{\eta_h \in \mathring{V}_h}{\operatorname{argmin}} \hat{E}(\eta_h, u_h^{n-1})$ . The unique solvability and energy stability (2.13) then follows from the similar argument in Theorem 2.1.  $\square$

**2.2. Convex splitting schemes and their equivalence to fully implicit schemes.** As we have seen before, convexity is a very desirable property of the discretize scheme and fully implicit scheme is only convex when  $k$  is sufficiently small. When  $k$  is not sufficiently small, the non-convexity of the discrete scheme comes from the fact that the potential function  $F$  in (1.3) is not convex. The convex splitting scheme (CSS in short) stems from splitting the non-convex potential function  $F$  given by (1.3) into the difference between two convex functions:

$$(2.16) \quad F(u) = F_+(u) - F_-(u), \quad \text{with} \quad F_+(u) = \frac{1}{4}(u^4 + 1), \quad F_-(u) = \frac{1}{2}u^2.$$

**2.2.1. A convex splitting scheme for the Allen-Cahn model.** In view of Theorem 2.1, a CSS be obtained by making the non-convex part, namely  $F_-(\cdot)$  in (2.16), explicit in some way, and it can be characterized by the minimization of a convex functional:

$$(2.17) \quad u_h^n = \operatorname{argmin}_{v \in V_h} \left\{ \int_{\Omega} \left( \frac{1}{2} |\nabla v|^2 + \frac{1}{\epsilon^2} [F_+(v) - \hat{F}_-(u_h^{n-1}, v)] \right) dx + \frac{1}{2k} \int_{\Omega} (v - u_h^{n-1})^2 dx \right\}$$

where  $\hat{F}_-(u_h^{n-1}, v)$  is the linearization of  $F_-(\cdot)$  at  $u_h^{n-1}$ , that is,  $\hat{F}_-(u_h^{n-1}, v) = F_-(u_h^{n-1}) + F'_-(u_h^{n-1})(v - u_h^{n-1})$ .

The variational formulation of (2.17) is the following well-known CSS: Find  $u_h^n \in V_h$  for  $n = 1, 2, \dots, N$ , such that

$$(2.18) \quad \left( \frac{u_h^n - u_h^{n-1}}{k}, v_h \right) + (\nabla u_h^n, \nabla v_h) + \frac{1}{\epsilon^2} ((u_h^n)^3 - u_h^{n-1}, v_h) = 0 \quad \forall v_h \in V_h.$$

**THEOREM 2.3.** [15] *The CSS scheme (2.18) is unconditionally energy stable.* At the first glance, the above result looks incredibly remarkable. As we have seen above, even a fully implicit scheme can not be unconditionally energy-stable, but as a partially implicit (or explicit) scheme, CSS is unconditionally energy-stable. Although, as we discussed before, we can not quite relate the energy-stability in a nonlinear scheme to the standard stability concept in a standard linear scheme, it is quite incredible that a partially implicit (or explicit) scheme is actually more stable than a fully implicit scheme!

This remarkable phenomenon can be explained by the following result.

**THEOREM 2.4.** *The CSS (2.18) can be recast as the FIS (2.2) with different time step size:*

$$(2.19) \quad k' = \frac{\epsilon^2}{k + \epsilon^2} k.$$

*Proof.* We write that

$$(u_h^n)^3 - u_h^{n-1} = f(u_h^n) + (u_h^n - u_h^{n-1}).$$

Substituting the above identity into (2.18) and regrouping the term involving  $u_h^n - u_h^{n-1}$ , we obtain

$$(2.20) \quad \left( \left( \frac{1}{k} + \frac{1}{\epsilon^2} \right) (u_h^n - u_h^{n-1}), v_h \right) + (\nabla u_h^n, \nabla v_h) + \frac{1}{\epsilon^2} (f(u_h^n), v_h) = 0 \quad \forall v_h \in V_h,$$

which is exactly the FIS with time step size (2.19).  $\square$

By comparing the condition for the time step size in Theorem 2.1 and (2.19), the resulting time-step constraint (2.19) in the CSS is actually more stringent to assure the convexity of the

original FIS, as  $k' < \epsilon^2$  for any  $\epsilon > 0$ . This also explains why the CSS is always energy-stable thanks to the Theorem 2.1.

REMARK 2.5. We now make some remark on the implication of Theorem 2.4. Let  $u_h^{\text{FIS}}(t_n)$  be the solution to (2.2) and  $u_h^{\text{CSS}}(t_n)$  be the solution to (2.18). Then by Theorem 2.4, we have

$$(2.21) \quad u_h^{\text{CSS}}(t_n) = u_h^{\text{FIS}}(\delta t_n), \quad \text{with} \quad \delta = \frac{\epsilon^2}{k + \epsilon^2}.$$

Here,  $\delta$  can be regarded as a delaying factor. A larger time step size  $k$ , which gives a smaller  $\delta$ , leads to a more significant time-delay. Even for a very small  $k$ , such a delay is not negligible. For example, if  $k = \epsilon^2$ , we have  $\delta = 1/2$ . Thus,  $u_h^{\text{CSS}}(t_n) = u_h^{\text{FIS}}(\frac{t_n}{2})$ .

Because of such a delay, it is expected and also numerically verified that, quantitatively speaking, the CSS may have a reduced accuracy although it gives qualitatively correct answer. Furthermore such a delay will diminish as  $k \rightarrow 0$  since  $\lim_{k \rightarrow 0} \delta = 1$ .

In summary, we conclude that the CSS has a special property that may be known as “delayed convergence” in the following sense:

1. The CSS scheme is expected to eventually converge to the exact solution of the originally Allen-Cahn equation as  $k \rightarrow 0$ .
2. But for any given time step size  $k$ , the CSS would approximate better the exact solution at a delayed time.

Test 1. In this test, the square domain  $\Omega = (-1, 1)^2$  is used to investigate the performance of different numerical schemes, and the initial condition is chosen as

$$(2.22) \quad u_0 = \tanh\left(\frac{d_0(x)}{\sqrt{2}\epsilon}\right).$$

Here,  $d_0(x)$  is the signed distance function from  $x$  to the initial curve  $\Gamma_0 : x^2 + y^2 = 0.6^2$ , i.e.,  $d_0(x) = \sqrt{x^2 + y^2} - 0.6$ . Figure 2.1 and 2.2 displays the evolution of the radius with respect to time. The singularity happens at  $t = 0.18$ , which is the disappearing time.

The numerical solutions of FIS and CSS with different  $h$ 's are plotted in 2.1. When decreasing  $h$ , the FIS approximates the exact solution well, while the CSS does not. The similar phenomenon happens with different  $\epsilon$ 's, as shown in Figure 2.2.

**2.2.2. A convex splitting scheme for the Cahn-Hilliard model.** Similar to the Allen-Cahn model, a convex splitting scheme can also be obtained for Cahn-Hilliard model as follows: Find  $u_h^n \in V_h$  for  $n = 1, 2, \dots, N$ , such that

$$(2.23) \quad \begin{aligned} & \left( \frac{u_h^n - u_h^{n-1}}{k}, \eta_h \right) + (\nabla w_h^n, \nabla \eta_h) = 0 \quad \forall \eta_h \in V_h, \\ & \epsilon (\nabla u_h^n, \nabla v_h) + \frac{1}{\epsilon} ((u_h^n)^3 - u_h^{n-1}, v_h) - (w_h^n, v_h) = 0 \quad \forall v_h \in V_h. \end{aligned}$$

THEOREM 2.6. The Discretization of the Cahn-Hilliard equation using the convex splitting scheme is equivalent to the discretization of the following equations using the fully implicit scheme:

$$(2.24) \quad \begin{aligned} & u_t - \Delta w = 0, \\ & w + \epsilon \Delta u - \frac{1}{\epsilon} f(u) - \frac{k}{\epsilon} u_t = 0. \end{aligned}$$

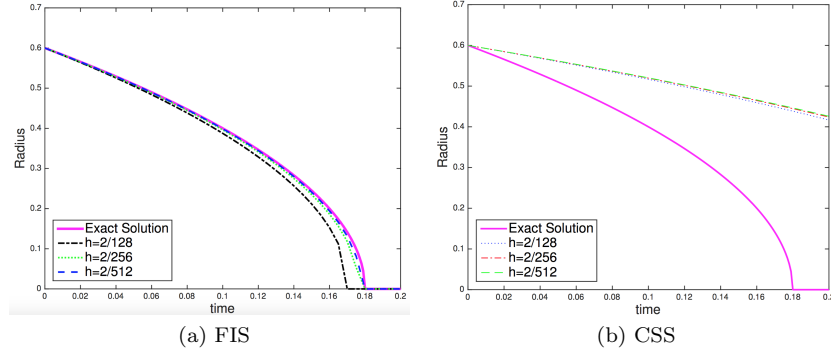


Fig. 2.1: Allen-Cahn equation: FIS and CSS with  $\epsilon = 0.02$ ,  $k = 0.0005$  and different  $h$ 's.

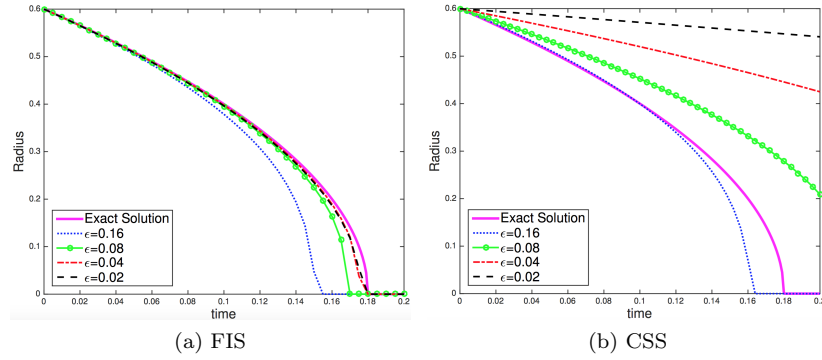


Fig. 2.2: Allen-Cahn equation: FIS and CSS with  $k = 0.002$ ,  $h = 1/256$  and different  $\epsilon$ 's.

We note that (2.24) can be equivalently written as follows:

$$(2.25) \quad \left(1 - \frac{k}{\epsilon}\Delta\right)u_t + \Delta(\epsilon\Delta u - \frac{1}{\epsilon}f(u)) = 0.$$

It is known that [9] when  $k = \mathcal{O}(\epsilon^3)$ , the solution of (2.25) converges to the Hele-Shaw flow, which is also the limiting dynamics for the Cahn-Hilliard equation (1.2). In other situations, for example, when  $k = \mathcal{O}(\epsilon^2)$ , their limiting dynamics may be different.

*Test 2.* In this test, the same domain is chosen as in Test 1, and the following initial condition for the Cahn-Hilliard equation is chosen as

$$(2.26) \quad u(x, t) = \tanh\left(\frac{\sqrt{x^2 + y^2} - 0.2}{\sqrt{2}\epsilon}\right), \quad \epsilon = 0.02.$$

Again, the Figure 2.3 is the snapshot showing the lagging phenomenon at different time points.



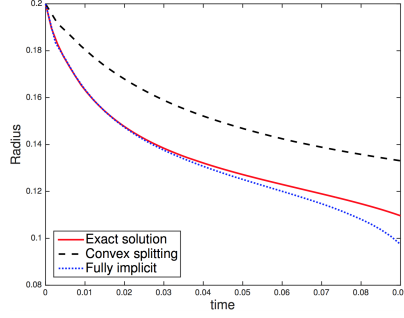


Fig. 2.3: Cahn-Hilliard equations: FIS and CSS. Here,  $\epsilon = 0.02$ ,  $k = 5 \times 10^{-4}$  and  $h = 0.015$ .

**2.3. Some other first-order partially implicit schemes.** In this section, we briefly discuss several other first-order partially implicit schemes for the Allen-Cahn model.

*Semi-implicit scheme:* Seeking  $u_h^n \in V_h$  for  $n = 1, 2, \dots, N$ , such that

$$(2.27) \quad \left( \frac{u_h^n - u_h^{n-1}}{k}, v_h \right) + (\nabla u_h^n, \nabla v_h) + \frac{1}{\epsilon^2} (f(u_h^{n-1}), v_h) = 0 \quad \forall v_h \in V_h.$$

*Stabilized semi-implicit scheme:* Seeking  $u_h^n \in V_h$  for  $n = 1, 2, \dots, N$ , such that

$$(2.28) \quad \left( \frac{1}{k} + \frac{S}{\epsilon^2} \right) (u_h^n - u_h^{n-1}, v_h) + (\nabla u_h^n, \nabla v_h) + \frac{1}{\epsilon^2} (f(u_h^{n-1}), v_h) = 0 \quad \forall v_h \in V_h,$$

where  $S > 0$  (set as  $S = 1$  in the Test 3) is a stabilized constant.

**THEOREM 2.7.** *The scheme (2.27) and (2.28) can be recast as*

$$(2.29) \quad \left( \frac{1 + \gamma_n}{k} (u_h^n - u_h^{n-1}), v_h \right) + (\nabla u_h^n, \nabla v_h) + \frac{1}{\epsilon^2} (f(u_h^n), v_h) = 0 \quad \forall v_h \in V_h.$$

For semi-implicit scheme (2.27),

$$\gamma_n = \frac{k}{\epsilon^2} [1 - (u_h^n)^2 - u_h^n u_h^{n-1} - (u_h^{n-1})^2],$$

and for stabilized semi-implicit scheme (2.28),

$$\gamma_n = \frac{k}{\epsilon^2} [1 + S - (u_h^n)^2 - u_h^n u_h^{n-1} - (u_h^{n-1})^2].$$

*Proof.* For semi-implicit and stabilized semi-implicit schemes, the parameter  $\delta_n$  can be derived from  $f(u_h^{n-1}) = f(u_h^n) + [1 - (u_h^n)^2 - u_h^n u_h^{n-1} - (u_h^{n-1})^2](u_h^n - u_h^{n-1})$ .  $\square$

Depending on the size and sign of  $\gamma_n$ , the above theorem will offer some insight to the behavior of the two semi-implicit schemes in comparison with the fully implicit scheme (2.2).

*Test 3.* In this test, the same domain and initial conditions are chosen as in Test 1. On the left graph of Figure 2.4, the same  $\epsilon$ ,  $h$  and  $k$  are chosen to draw the graphs using different numerical schemes comparing with the exact solution (which is obtained by highly refined meshes and extremely small time step size). We observe that only the FIS performs well. The right graph shows the delayed convergence" of the CSS.

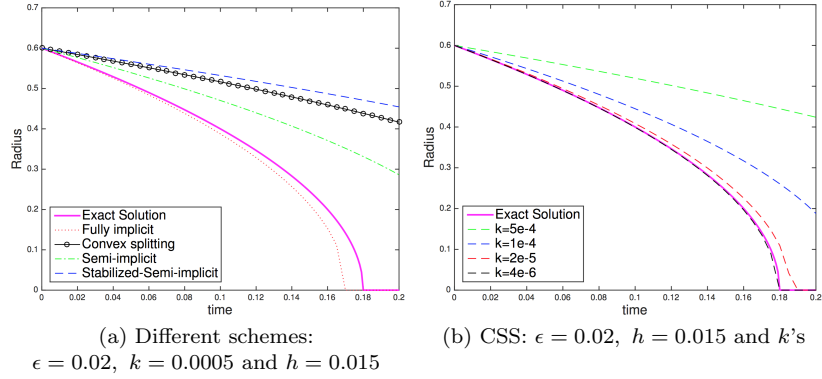


Fig. 2.4: Allen-Cahn equation: Radius change with time using different numerical methods.

**2.4. Convex splitting schemes interpreted as artificial convexity schemes.** In this section, we give a slightly different perspective on convex splitting schemes. We consider the following modified Allen-Cahn model:

$$(2.30) \quad \left(1 + \frac{\delta}{\epsilon^2}\right) u_t - \Delta u + \frac{1}{\epsilon^2} f(u) = 0,$$

and the following modified Cahn-Hilliard model:

$$(2.31) \quad \begin{aligned} \left(1 - \frac{\delta}{\epsilon} \Delta\right) u_t - \Delta w &= 0 & \text{in } \Omega_T, \\ -\epsilon \Delta u + \frac{1}{\epsilon} f(u) &= w & \text{in } \Omega_T. \end{aligned}$$

**THEOREM 2.8.** *When  $k \leq \epsilon^2 + \delta$ , the standard fully implicit scheme for (2.30) is equivalent to the convex minimization problem:*

$$(2.32) \quad u_h^n = \operatorname{argmin}_{v_h \in V_h} \left\{ J_\epsilon^{AC}(v) + \left(\frac{1}{2k} + \frac{\delta}{2k\epsilon^2}\right) \int_\Omega (u - u_h^{n-1})^2 dx \right\}.$$

*When  $k \leq (\epsilon^{3/2} + \sqrt{\epsilon^3 + \delta})^2$ , the standard fully implicit scheme for (2.31) is equivalent to the convex minimization problem:*

$$(2.33) \quad u_h^n = u_h^{n-1} + \theta_h, \quad \theta_h = \operatorname{argmin}_{v_h \in \tilde{V}_h} \left\{ J_\epsilon^{CH}(u_h^{n-1} + \theta_h) + \frac{1}{2k} \|\nabla \Delta_h^{-1} \theta_h\|_{L^2(\Omega)}^2 + \frac{\delta}{2k\epsilon} \|\theta_h\|_{L^2(\Omega)}^2 \right\}.$$

*Proof.* The proofs of (2.32) and (2.33) are similar to Theorem 2.1 and 2.2, respectively.  $\square$

In view of Theorem 2.8, the modified model (2.30) may be viewed as a convexified model of the original Allen-Cahn model (1.1); the added term  $\frac{\delta}{\epsilon^2} u_t$  introduces a new time scale of the model and on the discrete level it plays the role of an artificial convexification. Similarly, the modified

model (2.31) may be viewed as a convexified model of the original Cahn-Hilliard model (1.2). We note that the CSS for the original Allen-Cahn or Cahn-Hilliard model is the FIS for the convexified model with  $\delta = k$ .

With such an interpretation, the convex splitting scheme may be more appropriately viewed as an artificial convexity scheme. This is in some way similar to the artificial viscosity scheme for hyperbolic equations or convection dominated convection-diffusion problems. The physical implication of the convexified model (2.30) is a new time-scale:  $t' = (1 + \frac{\delta}{\epsilon^2})t$ , which leads to a time-delay in comparison to the original model. The implication of the modified model (2.31) seems to be similar but less obvious.

**3. A modified FIS satisfying a discrete maximum principle.** In this section, we will modify the fully implicit scheme (or the corresponding convex splitting scheme) to preserve the maximum principle on discrete level. We will then further show that this modified scheme can be uniformly preconditioned by a Poisson-like operator. We refer to [27, 32] for other maximum principle preserving schemes for the Allen-Cahn equation.

**3.1. A modified scheme.** Our modified FIS is motivated by the maximum principle of Allen-Cahn on continuous level stated in the following theorem (see [12, 16] for the idea, and Proposition 2.2.1 in [25] for the details).

**THEOREM 3.1.** *If  $u$  is a weak solution of the Allen-Cahn equation (1.1) and  $\|u_0\|_{L^\infty(\Omega)} \leq 1$ , then  $\|u(x, t)\|_{L^\infty(\Omega)} \leq 1$ . Unfortunately, the above maximum principle can not be proved for a standard FIS. In this section, we will modify the standard FIS scheme so that a maximum principle preserving scheme analogous to Theorem 3.1 can also be rigorously proved.*

We consider the  $P_1$ -Lagrangian finite element space in this section,

$$V_h = \{v_h \in C(\bar{\Omega}) : v_h|_K \in P_1(K)\}.$$

The nodal basis function of  $V_h$  related to the vertex  $a_i$  is denoted as  $\varphi_i$ . We then define the nodal value interpolation  $I_h : C(\bar{\Omega}) \mapsto V_h$  as

$$(3.1) \quad I_h v := \sum_{a_i \in \mathcal{N}_h} v(a_i) \varphi_i = \sum_{a_i \in \mathcal{N}_h} v_i \varphi_i.$$

Following [38], for given  $K \in \mathcal{T}_h$ , we introduce the following notation:  $a_i (1 \leq i \leq n+1)$  denote the vertices of  $K$ ,  $E = E_{ij}$  the edge connecting two vertices  $a_i$  and  $a_j$ ,  $F_i$  the  $(n-1)$ -dimensional simplex opposite to the vertex  $a_i$ ,  $\theta_{ij}^K$  or  $\theta_E^K$  the angle between the faces  $F_i$  and  $F_j$ ,  $\kappa_E^K = F_i \cap F_j$ , the  $(n-2)$ -dimensional simplex opposite to the edge  $E = E_{ij}$ .

We first consider the simplest and important case of the Poisson equation with Neumann boundary condition. Then, for any  $u_h, v_h \in V_h$ , we have (see [38] for details)

$$(3.2) \quad (\nabla u_h, \nabla v_h) = \sum_{K \in \mathcal{T}_h} \sum_{E \subset K} \omega_E^K \delta_E u_h \delta_E v_h,$$

where  $\delta_E \phi = \phi(a_i) - \phi(a_j)$  for any continuous function  $\phi$  on  $E = E_{ij}$  and  $\omega_E^K = \frac{1}{n(n-1)} |\kappa_E^K| \cot \theta_E^K$ . We will make the following assumption

$$(3.3) \quad w_E := \frac{1}{n(n-1)} \sum_{K \supset E} |\kappa_E^K| \cot \theta_E^K \geq 0 \quad \text{for any edge } E.$$

We note that, in 2D, the above assumption (3.3) is equivalent to the Delaunay condition [35] which requires the sum of any pair of angles facing a common interior edge to be less than or equal to  $\pi$ . For higher dimension a sufficient condition on  $\mathcal{T}_h$  for (3.3) that all the angles between any two adjacent  $(n-1)$ -simplices from  $\mathcal{T}_h$  are less than or equal to  $\frac{\pi}{2}$ .

With the help of nodal value interpolation, we define a norm  $\|\cdot\|_h$  on  $V_h$  as

$$(3.4) \quad \|v_h\|_h^2 := \int_{\Omega} I_h(v_h^2) \, dx.$$

Our *modified FIS* is as follows: Find  $u_h^n \in V_h$  for  $n = 1, 2, \dots, N$ , such that

$$(3.5) \quad \left(\frac{1}{k} I_h((u_h^n - u_h^{n-1})v_h), 1\right) + (\nabla u_h^n, \nabla v_h) + \frac{1}{\epsilon^2} (I_h(f(u_h^n)v_h), 1) = 0 \quad \forall v_h \in V_h.$$

**THEOREM 3.2.** *Assume the triangulation satisfies (3.3). If  $u_h^n$  is a solution of the modified FIS (3.5) and  $\|u_h^0\|_{L^\infty(\Omega)} \leq 1$ , then  $\|u_h^n\|_{L^\infty(\Omega)} \leq 1$ , for all  $n \geq 0$ .*

*Proof.* For any function  $v \in C(\bar{\Omega})$ , we introduce the following notation:

$$v^+ = \begin{cases} v & \text{if } v \geq 0, \\ 0 & \text{otherwise,} \end{cases} \quad \text{and} \quad v^- = \begin{cases} -v & \text{if } v \leq 0, \\ 0 & \text{otherwise.} \end{cases}$$

A quick calculation shows that for any  $v_i, v_j$ ,

$$(v_i - v_j)(v_i^+ - v_j^+) - (v_i^+ - v_j^+)^2 = -(v_i^+ - v_j^+)(v_i^- - v_j^-) \geq 0.$$

Therefore, the (3.2) and (3.3) imply

$$\begin{aligned} (\nabla v_h, \nabla I_h(v_h^+)) &= \sum_{K \in \mathcal{T}_h} \sum_{E \subset K} w_E^K \delta_E v_h \delta_E (I_h(v_h^+)) \\ &\geq \sum_{K \in \mathcal{T}_h} \sum_{E \subset K} w_E^K \delta_E (I_h(v_h^+)) \delta_E (I_h(v_h^+)) = \|\nabla I_h(v_h^+)\|_{L^2(\Omega)}^2. \end{aligned}$$

This proves that

$$(3.6) \quad (\nabla v_h, \nabla I_h(v_h^+)) \geq \|\nabla I_h(v_h^+)\|_{L^2(\Omega)}^2.$$

We now finish the proof by induction. First, the result holds for  $n = 0$  by assumption. Assume the result holds for  $n - 1$ , i.e.  $\|u_h^{n-1}\|_{L^\infty(\Omega)} \leq 1$ . Then, we define a special test function  $v_h \in V_h$  as  $v_h := I_h((u_h^n - 1)^+)$ . Notice that  $\|u_h^{n-1}\|_{L^\infty(\Omega)} \leq 1$  implies

$$\frac{1}{k}(u_h^n - u_h^{n-1}) \geq \frac{1}{k}(u_h^n - 1),$$

which means that

$$\begin{aligned} \left(\frac{1}{k} I_h((u_h^n - u_h^{n-1})v_h), 1\right) &= \frac{1}{k} \int_{\Omega} I_h((u_h^n - u_h^{n-1})(u_h^n - 1)^+) \, dx \\ &\geq \frac{1}{k} \int_{\Omega} I_h((u_h^n - 1)(u_h^n - 1)^+) = \frac{1}{k} \|I_h((u_h^n - 1)^+)\|_h^2. \end{aligned}$$

Furthermore by (3.6) and the inductive assumption,

$$\begin{aligned} (\nabla u_h^n, \nabla v_h) &= (\nabla(u_h^n - 1), \nabla I_h((u_h^n - 1)^+)) \geq \|\nabla I_h((u_h^n - 1)^+)\|_{L^2(\Omega)}^2 \geq 0, \\ (I_h(f(u_h^n)v_h), 1) &= \int_{\Omega} I_h((u_h^n + 1)u_h^n(u_h^n - 1)(u_h^n - 1)^+) dx \geq 0. \end{aligned}$$

Therefore,

$$\frac{1}{k} \|I_h((u_h^n - 1)^+)\|_h^2 \leq (\frac{1}{k} I_h((u_h^n - u_h^{n-1})v_h), 1) + (\nabla u_h^n, \nabla v_h) + \frac{1}{\epsilon^2} (I_h(f(u_h^n)v_h), 1) = 0,$$

which implies  $I_h((u_h^n - 1)^+) = 0$ , thus  $u_h^n \leq 1$ . Similarly, by choosing a special test function  $v_h := I_h((u_h^n + 1)^-)$ , we can prove that  $u_h^n \geq -1$ . Therefore,  $\|u_h^n\|_{L^\infty(\Omega)} \leq 1$ .  $\square$

*Test 4.* In this test, the same domain is chosen as in Test 1, and the random initial condition for the Allen-Cahn equation is used with  $\epsilon = 0.01$ . In Figure 3.1, it shows the random initial condition, the evolutions, and the  $L^\infty$ -norm of the numerical solutions at different time points.

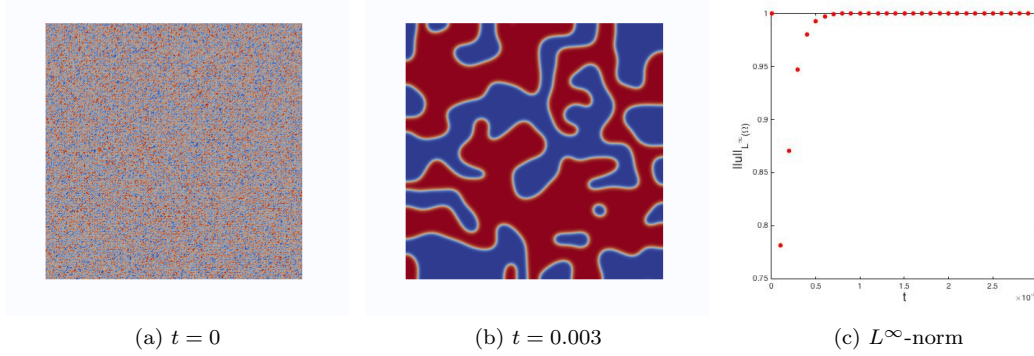


Fig. 3.1: Performance of modified FIS with random initial condition.

REMARK 3.3. *An analogous technique can be applied to prove the discrete maximum principle for the convex splitting scheme with mass lumping*

$$(3.7) \quad (\frac{1}{k} I_h((u_h^n - u_h^{n-1})v_h), 1) + (\nabla u_h^n, \nabla v_h) + \frac{1}{\epsilon^2} (I_h([(u_h^n)^3 - u_h^{n-1}]v_h), 1) = 0 \quad \forall v_h \in V_h.$$

*This comes from the fact that (3.7) can be considered as the (3.5) with the time step size  $\frac{\epsilon^2}{k+\epsilon^2}k$ .*

REMARK 3.4. *We define the modified free-energy functional and discrete energy*

$$\begin{aligned} J_{\epsilon, I}^{AC}(u) &= \int_{\Omega} \frac{1}{2} |\nabla u|^2 + \frac{1}{\epsilon^2} I_h(F(u)) dx, \\ E_I(u, u_h^{n-1}) &= J_{\epsilon, I}^{AC}(u) + \frac{1}{2k} \int_{\Omega} I_h(u - u_h^{n-1})^2 dx. \end{aligned}$$

*Similar to Theorem 2.1, we have the following result under the condition that  $k \leq \epsilon^2$ ,*

1.  $E_I(\cdot, u_h^{n-1})$  is strictly convex on  $H^1(\Omega)$ .
2. The equation (3.7) satisfies  $u_h^n = \underset{v_h \in V_h}{\operatorname{argmin}} E_I(v_h, u_h^{n-1})$ .
3. The following energy law holds

$$(3.8) \quad J_{\epsilon, I}^{AC}(u_h^n) + \frac{1}{2k} \|u_h^n - u_h^{n-1}\|_{L^2(\Omega)}^2 \leq J_{\epsilon, I}^{AC}(u_h^{n-1}).$$

**3.2. A robust preconditioner for the Allen-Cahn equation.** Next we will analyze a simple preconditioner for the Newton linearization of modified FIS (3.5). With this preconditioner, the resulting preconditioned conjugate gradient method (PCG) significantly reduces the number of iterations of the conjugate gradient method (CG), and moreover, the number of iterations is uniform with respect to the spatial meshes which can be locally refined. We acknowledge that some nonlinear multigrid methods have been applied to numerical schemes similar to (3.5) in the literature, see [24, 36, 37].

We first define the mass lumping operator  $\mathcal{I}_h[u] : V_h \mapsto V_h$  as

$$(3.9) \quad (\mathcal{I}_h[u]v_h, w_h) := (I_h(uv_hw_h), 1) \quad \forall v_h, w_h \in V_h, u \in C(\bar{\Omega}).$$

Let  $\mathcal{I}_h = \mathcal{I}_h[1]$  for convenience. The Fréchet derivative of scheme (3.5) is denoted by  $\mathcal{L}_h[u_h^n] : V_h \mapsto V_h$ , such that

$$(3.10) \quad (\mathcal{L}_h[u_h^n]v_h, w_h) := \left(\frac{1}{k}\mathcal{I}_h v_h, w_h\right) - (\Delta_h v_h, w_h) + \frac{1}{\epsilon^2} (\mathcal{I}_h[(3u_h^n)^2 - 1]v_h, w_h) \quad \forall v_h, w_h \in V_h.$$

**THEOREM 3.5.** *The upper and lower bounds of  $\mathcal{L}_h[u_h^n]$  are given by*

$$(3.11) \quad \frac{1-\gamma}{k}\mathcal{I}_h - \Delta_h \leq \mathcal{L}_h[u_h^n] \leq \frac{1+2\gamma}{k}\mathcal{I}_h - \Delta_h.$$

where  $\gamma := k/\epsilon^2$ .

*Proof.* In light of (3.10), we only need to prove

$$-\gamma(\mathcal{I}_h v_h, v_h) \leq \frac{k}{\epsilon^2} (I_h([(3u_h^n)^2 - 1](v_h)^2), 1) \leq 2\gamma(\mathcal{I}_h v_h, v_h) \quad \forall v_h \in V_h.$$

The left inequality can be proved by fact that  $3(u_h^n)^2 - 1 \geq -1$ , and the right inequality can be proved by the fact that  $3(u_h^n)^2 - 1 \leq 2$  due to the discrete maximum principle in Theorem 3.2.  $\square$

Based on the Theorem 3.5, it is an immediate consequence that when  $\gamma \leq 1$ , or  $k \leq \epsilon^2$ ,  $(\mathcal{L}_h[u_h^n]v_h, v_h) \geq 0$  for any  $v_h \in V_h$ , which implies the convexity of the discrete energy with mass lumping  $\tilde{E}(\cdot, u_h^{n-1})$ :

$$\tilde{E}(u, u_h^{n-1}) := \frac{1}{\epsilon^2} \int_{\Omega} I_h(F(u)) \, dx + \frac{1}{2k} \int_{\Omega} I_h((u - u_h^{n-1})^2) + \frac{1}{2} \|\nabla u\|_{L^2(\Omega)}^2.$$

Thus, the uniqueness and existence of FIS with mass lumping hold when  $k \leq \epsilon^2$ . Further, we can design a preconditioner for  $\mathcal{L}_h[u_h^n]$  as

$$(3.12) \quad \mathcal{B}_h = \left( \frac{1-\gamma}{k}\mathcal{I}_h - \Delta_h \right)^{-1}.$$

Then, we have the following theorem directly followed from the Theorem 3.5.

**THEOREM 3.6.** *It holds that*

$$(3.13) \quad \kappa(\mathcal{B}_h \mathcal{L}_h[u_h^n]) \leq \frac{1+2\gamma}{1-\gamma}.$$

**REMARK 3.7.** *When the uniform meshes are used with  $h^{-1} = \mathcal{O}(\epsilon^{-1})$  and  $k = \mathcal{O}(\epsilon^2)$ , then it is apparent that  $\mathcal{L}_h[u_h^n]$  is already well-conditioned. Therefore, the above Theorem 3.6 is of special interest when the adaptive meshes are used.*

*Test 5.* In this test, consider the initial condition (2.26) and the scheme (3.5), and  $\epsilon = 0.02$ ,  $k = \frac{\epsilon^2}{2} = 2 \times 10^{-4}$ . The simulation on adaptive meshes is partially based on the MATLAB software package *iFEM* [6], and the mesh refining and coarsening are based on the error estimator in [20]. The adaptive tolerance is  $10^{-5}$  and the maximal bisection level  $J = 20$ . When the maximal bisection level increases, the number of degrees of freedom (DOF) increases, then the numbers of iterations of CG and PCG are compared in the Table 3.1 to verify the theoretical results.

DOF	301	368	430	510	566	672	1276	1633	2044	2535	3217	4027	4610
CG	21	32	37	38	41	45	58	61	68	78	96	106	117
PCG	9	8	8	9	8	8	8	8	8	8	8	8	8

Table 3.1: The number of iterations for CG and PCG.

**4. Second-order schemes.** In this section, we shall consider the second-order schemes.

**4.1. (Modified) Crank-Nicolson scheme for the Allen-Cahn equation.** The standard Crank-Nicolson scheme for the Allen-Cahn equation, is to seek  $u_h^n \in V_h$  for  $n = 1, 2, \dots, N$ , such that

$$(4.1) \quad \left( \frac{u_h^n - u_h^{n-1}}{k}, v_h \right) + \left( \frac{\nabla u_h^n + \nabla u_h^{n-1}}{2}, \nabla v_h \right) + \frac{1}{2\epsilon^2} (f(u_h^n) + f(u_h^{n-1}), v_h) = 0 \quad \forall v_h \in V_h,$$

Although the standard Crank-Nicolson scheme can not be proved energy stable, in view of (4.1), we can still show its convexity by defining the following discrete energy

$$(4.2) \quad \bar{E}(u, u_h^{n-1}) = \frac{1}{4} \|\nabla u\|_{L^2(\Omega)}^2 + \frac{1}{2} (\nabla u, \nabla u_h^{n-1}) + \frac{1}{2k} \|u - u_h^{n-1}\|_{L^2(\Omega)}^2 + \frac{1}{\epsilon^2} \int_{\Omega} \bar{G}(u, u_h^{n-1}) \, dx,$$

where  $\bar{G}(u, u_h^{n-1}) = \bar{G}_+(u, u_h^{n-1}) - \bar{G}_-(u, u_h^{n-1})$ , and

$$\bar{G}_+(u, u_h^{n-1}) = \frac{1}{2} \left[ \frac{1}{4} u^4 + (u_h^{n-1})^3 u \right] \quad \text{and} \quad \bar{G}_-(u, u_h^{n-1}) = \frac{1}{4} u^2 + \frac{1}{2} u u_h^{n-1}.$$

**THEOREM 4.1.** *Under the condition that  $k \leq 2\epsilon^2$ , we have*

1.  $\bar{E}(v_h, u_h^{n-1})$  is strictly convex on  $V_h$ ;
2. The solution of the modified Crank-Nicolson scheme (4.1) satisfies

$$u_h^n = \operatorname{argmin}_{v_h \in V_h} \bar{E}(v_h, u_h^{n-1}),$$

*which is uniquely solvable.*

*Proof.* A direct calculation shows that

$$\bar{\bar{E}}''(u, u_h^{n-1})(v_h, v_h) = \frac{1}{2} \|\nabla v_h\|_{L^2(\Omega)}^2 + \left(\frac{1}{k} - \frac{1}{2\epsilon^2}\right) \|v_h\|_{L^2(\Omega)}^2 + \frac{1}{2\epsilon^2} \int_{\Omega} 3u^2 v_h^2 \, dx.$$

This implies that  $\bar{\bar{E}}(\cdot, u_h^{n-1})$  is a strictly convex functional when  $k \leq 2\epsilon^2$ . The rest of the proof is standard.  $\square$

With the purpose of energy stability, the *modified Crank-Nicolson scheme* [13, 33, 11] is constructed as follows: Find  $u_h^n \in V_h$  for  $n = 1, 2, \dots, N$ , such that

$$(4.3) \quad \left(\frac{u_h^n - u_h^{n-1}}{k}, v_h\right) + \left(\frac{\nabla u_h^n + \nabla u_h^{n-1}}{2}, \nabla v_h\right) + \frac{1}{\epsilon^2} (\tilde{F}(u_h^n, u_h^{n-1}), v_h) = 0 \quad \forall v_h \in V_h,$$

where

$$\tilde{F}(u, u_h^{n-1}) = \begin{cases} \frac{F(u) - F(u_h^{n-1})}{u - u_h^{n-1}} & u \neq u_h^{n-1}, \\ u^3 - u & u = u_h^{n-1}. \end{cases}$$

LEMMA 4.2 ([33, 11]). *The modified Crank-Nicolson scheme (4.3) is unconditionally energy stable. More precisely, for any  $k > 0$ ,*

$$(4.4) \quad J_{\epsilon}^{AC}(u_h^n) + \frac{1}{k} \|u_h^n - u_h^{n-1}\|_{L^2(\Omega)}^2 = J_{\epsilon}^{AC}(u_h^{n-1}).$$

*Proof.* (4.4) is an immediate consequence by taking  $v_h = u_h^n - u_h^{n-1}$  in (4.3).  $\square$

The modified Crank-Nicolson scheme (4.3) is unconditionally energy-stable but it is not unconditionally convex as we shall see below. In view of (4.3), we define the following discrete energy

$$(4.5) \quad \tilde{E}(u, u_h^{n-1}) = \frac{1}{4} \|\nabla u\|_{L^2(\Omega)}^2 + \frac{1}{2} (\nabla u, \nabla u_h^{n-1}) + \frac{1}{2k} \|u - u_h^{n-1}\|_{L^2(\Omega)}^2 + \frac{1}{\epsilon^2} \int_{\Omega} \check{G}(u, u_h^{n-1}) \, dx,$$

where  $\check{G}(u, u_h^{n-1}) = \check{G}_+(u, u_h^{n-1}) - \check{G}_-(u, u_h^{n-1})$ , and

$$\check{G}_+(u, u_h^{n-1}) = \frac{1}{4} \left[ \frac{1}{4} u^4 + \frac{u_h^{n-1}}{3} u^3 + \frac{(u_h^{n-1})^2}{2} u^2 + (u_h^{n-1})^3 u \right] \quad \text{and} \quad \check{G}_-(u, u_h^{n-1}) = \frac{1}{4} u^2 + \frac{1}{2} u u_h^{n-1}.$$

THEOREM 4.3. *Under the condition that  $k \leq 2\epsilon^2$ , we have*

1.  $\tilde{E}(v_h, u_h^{n-1})$  is strictly convex on  $V_h$ ;
2. The solution of the modified Crank-Nicolson scheme (4.3) satisfies

$$u_h^n = \underset{v_h \in V_h}{\operatorname{argmin}} \tilde{E}(v_h, u_h^{n-1}),$$

which is uniquely solvable.

*Proof.* A direct calculation shows that

$$\tilde{E}''(u, u_h^{n-1})(v_h, v_h) = \frac{1}{2} \|\nabla v_h\|_{L^2(\Omega)}^2 + \left(\frac{1}{k} - \frac{1}{2\epsilon^2}\right) \|v_h\|_{L^2(\Omega)}^2 + \frac{1}{4\epsilon^2} \int_{\Omega} [3u^2 + 2u_h^{n-1}u + (u_h^{n-1})^2] v_h^2 \, dx.$$



This implies that  $\tilde{E}(\cdot, u_h^{n-1})$  is a strictly convex functional when  $k \leq 2\epsilon^2$ . The rest of the proof is standard.  $\square$  The “convexity size” of standard and modified Crank-Nicolson schemes are the same. We also observe the similar numerical performance of these two schemes (see Test 6 below), although the standard Crank-Nicolson does not satisfy the energy stability.

REMARK 4.4. *Similar to the CSS (2.18), we can obtain the corresponding convex splitting version of the modified Crank-Nicolson scheme in the following:*

$$(4.6) \quad \left(\frac{u_h^n - u_h^{n-1}}{k}, v_h\right) + \left(\frac{\nabla u_h^n + \nabla u_h^{n-1}}{2}, \nabla v_h\right) + \frac{1}{\epsilon^2} (g_+(u_h^n, u_h^{n-1}) - g_-(u_h^{n-1}, u_h^{n-1}), v_h) = 0 \quad \forall v_h \in V_h.$$

where

$$g_+(u, u_h^{n-1}) = G'_+(u, u_h^{n-1}) = \frac{1}{4} [u^3 + u_h^{n-1}u^2 + (u_h^{n-1})^2u + (u_h^{n-1})^3],$$

$$g_-(u, u_h^{n-1}) = G'_-(u, u_h^{n-1}) = \frac{1}{2}(u + u_h^{n-1}).$$

Similar to Theorem 2.4, we know that the convex splitting scheme (4.6) can be recast as the modified Crank-Nicolson scheme (4.3) with the time step size  $k' = \frac{2\epsilon^2}{k+2\epsilon^2}k$ . This also shows the delay effect of the convex splitting scheme (4.6) and the original fully implicit scheme (4.3), but with a slightly different delay-factor:  $\delta = \frac{2\epsilon^2}{k+2\epsilon^2}$ .

Again, similar to the argument we made in § 2.2.1, the convex splitting scheme (4.6) derived here is nothing new but exactly the same as the original modified Crank-Nicolson scheme (4.3) in disguise with a reduced time step size.

**4.2. Modified Crank-Nicolson scheme for the Cahn-Hilliard equation.** The modified Crank-Nicolson scheme [13, 33, 11]. for the Cahn-Hilliard model is defined as follows: Find  $u_h^n \in V_h$ ,  $w_h^n \in V_h$  for  $n = 1, 2, \dots, n$  such that

$$(4.7) \quad \begin{aligned} \left(\frac{u_h^n - u_h^{n-1}}{k}, \eta_h\right) + (\nabla w_h^{n-\frac{1}{2}}, \nabla \eta_h) &= 0 \quad \forall \eta_h \in V_h, \\ \epsilon(\nabla u_h^{n-\frac{1}{2}}, \nabla v_h) + \frac{1}{\epsilon}(\tilde{F}(u_h^n, u_h^{n-1}), v_h) - (w_h^{n-\frac{1}{2}}, v_h) &= 0 \quad \forall v_h \in V_h. \end{aligned}$$

LEMMA 4.5 ([11, 33]). *The modified Crank-Nicolson scheme (4.7) is unconditionally energy stable. More precisely, for any  $k > 0$ ,*

$$(4.8) \quad J_\epsilon^{CH}(u_h^n) + \frac{1}{k} \|\nabla \Delta_h^{-1}(u_h^n - u_h^{n-1})\|_{L^2(\Omega)}^2 = J_\epsilon^{CH}(u_h^{n-1}).$$

*Proof.* It can be directly proved by taking  $\eta_h = \Delta_h^{-1}(u_h^n - u_h^{n-1})$  and  $v_h = u_h^n - u_h^{n-1}$  in (4.7).  $\square$

Consider the Cahn-Hilliard equation, we define the following discrete energy

$$(4.9) \quad \bar{E}(u, u_h^{n-1}) = \frac{\epsilon}{4} \|\nabla u\|_{L^2(\Omega)}^2 + \frac{\epsilon}{2} (\nabla u, \nabla u_h^{n-1}) + \frac{1}{2k} \|\nabla \Delta_h^{-1}(u - u_h^{n-1})\|_{L^2(\Omega)}^2 + \frac{1}{\epsilon} \int_\Omega G(u, u_h^{n-1}) \, dx,$$

where

$$(4.10) \quad G(u, u_h^{n-1}) = \frac{1}{4} \left[ \frac{1}{4} u^4 + \frac{u_h^{n-1}}{3} u^3 + \frac{(u_h^{n-1})^2}{2} u^2 + (u_h^{n-1})^3 u \right] - \frac{1}{4} u^2 - \frac{1}{2} u u_h^{n-1}.$$

**THEOREM 4.6.** *Under the assumption that  $k \leq 8\epsilon^3$ , we have*

1.  $\bar{E}(v_h, u_h^{n-1})$  is strictly convex on  $\dot{V}_h$ ;
2. The solution of the modified Crank-Nicolson scheme (4.7) satisfies

$$u_h^n = u_h^{n-1} + \theta_h, \quad \text{with } \theta_h = \underset{\eta_h \in \dot{V}_h}{\operatorname{argmin}} \bar{E}(\eta_h, u_h^{n-1}),$$

which is uniquely solvable.

*Proof.* By the definition of operator  $\Delta_h$  and the Schwarz's inequality, we have

$$(4.11) \quad \frac{1}{2\epsilon} \|v_h\|_{L^2(\Omega)}^2 \leq \frac{1}{8\epsilon^3} \|\nabla \Delta_h^{-1} v_h\|_{L^2(\Omega)}^2 + \frac{\epsilon}{2} \|\nabla v_h\|_{L^2(\Omega)}^2.$$

A direct calculation shows that

$$(4.12) \quad \begin{aligned} \bar{E}''(u, u_h^{n-1})(v_h, v_h) &= \frac{\epsilon}{2} \|\nabla v_h\|_{L^2(\Omega)}^2 + \frac{1}{k} \|\nabla \Delta_h^{-1} v_h\|_{L^2(\Omega)}^2 - \frac{1}{2\epsilon} \|v_h\|_{L^2(\Omega)}^2 \\ &\quad + \frac{1}{4\epsilon} \int_{\Omega} [3u^2 + 2u_h^{n-1}u + (u_h^{n-1})^2] v_h^2 dx. \end{aligned}$$

This implies that  $\bar{E}(\cdot, u_h^{n-1})$  is strictly convex when  $k \leq 8\epsilon^3$ . The rest of the proof is standard.  $\square$

**REMARK 4.7.** *Similar to the Allen-Cahn equation, the standard Crank-Nicolson can also be constructed and analyzed for the Cahn-Hilliard equations.*

**4.3. Some other second-order partially implicit schemes.** In this section, we briefly discuss several other second-order partially implicit schemes.

*Second-order stabilized semi-implicit scheme (BDF2):* Seeking  $u_h^n \in V_h$  for  $n = 1, 2, \dots, N$  such that

$$(4.13) \quad \begin{aligned} &\left( \frac{3u_h^n - 4u_h^{n-1} + u_h^{n-2}}{2k}, v_h \right) + (\nabla u_h^n, \nabla v_h) + \frac{1}{\epsilon^2} ((2f(u_h^{n-1}) - f(u_h^{n-2})), v_h) \\ &\quad + \frac{S}{\epsilon^2} (u_h^n - 2u_h^{n-1} + u_h^{n-2}, v_h) = 0 \quad \forall v_h \in V_h, \end{aligned}$$

where  $S > 0$  (set as  $S = 10$  in the Test 6) is a stabilized constant.

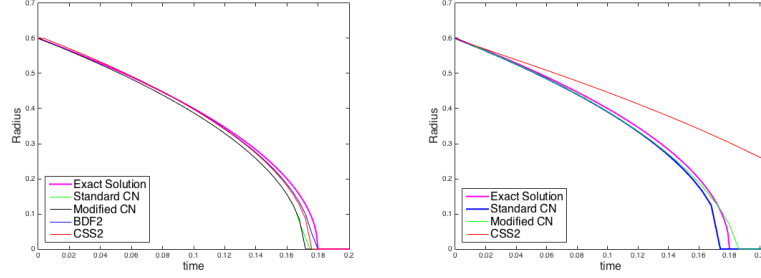
*Second-order convex splitting scheme (CSS2):* Seeking  $u_h^n \in V_h$  for  $n = 1, 2, \dots, N$ , such that

$$(4.14) \quad \left( \frac{u_h^n - u_h^{n-1}}{k}, v_h \right) + \left( \frac{\nabla u_h^n + \nabla u_h^{n-1}}{2}, \nabla v_h \right) + \frac{1}{\epsilon^2} (g_+(u_h^n, u_h^{n-1}) - \frac{1}{2\epsilon^2} (3u_h^{n-1} - u_h^{n-2}), v_h) = 0.$$

We know that BDF2 is a linear scheme so that satisfies the convexity property. Similar to the argument for the CSS version of modified Crank-Nicolson scheme (4.6), we know that (4.14) also satisfies the convexity property. When  $k \leq \epsilon^2$ , these second-order splitting schemes perform well (see Test 6 below). However, we observe the following phenomenon for these second-order splitting schemes:

1. They do not satisfy the discrete maximum principle, and it is frequently worse than the first-order scheme;
2. They still suffer the lagging phenomenon or delayed convergence for large time step size (see Test 6 below);

*Test 6.* In this test, the same domain and initial conditions are chosen as in Test 1. Figure 4.1a shows the evolution of the radius with respect to time for different second-order schemes. We observe that all these second-order schemes perform well when  $k = \epsilon^2$ . The performance of standard and modified Crank-Nicolson schemes are similar. When increasing the time step size, however, we observe that the lagging phenomenon exists for the CSS2 (see Figure 4.1b).



(a) Small time step:  $k = \epsilon^2 = 0.0004$       (b) Large time step:  $k = 15\epsilon^2 = 0.006$

Fig. 4.1: Different second-order schemes for Allen-Cahn:  $\epsilon = 0.02$ ,  $h = 0.015$ , and  $T = 0.2$

**4.4. Artificial convexity.** Following §2.4, the concept of artificial convexity scheme can also be applied to the widely used CSS2 (4.14) by considering the following modified model:

$$(4.15) \quad u_t + \frac{\delta}{\epsilon^2} u_{tt} - \Delta u + \frac{1}{\epsilon^2} f(u) = 0.$$

The modified Crank-Nicolson of (4.15) can be written as

$$\begin{aligned} \left( \frac{u_h^n - u_h^{n-1}}{k}, v_h \right) + \left( \frac{\delta}{\epsilon^2} \cdot \frac{u_h^n - 2u_h^{n-1} + u_h^{n-2}}{k^2}, v_h \right) \\ + \left( \frac{\nabla u_h^n + \nabla u_h^{n-1}}{2}, \nabla v_h \right) + \frac{1}{\epsilon^2} (\tilde{F}(u_h^n, u_h^{n-1}), v_h) = 0 \quad \forall v_h \in V_h, \end{aligned}$$

which is exactly the CSS2 scheme (4.14) when  $\delta = \frac{k^2}{2}$ .

**5. Concluding remarks.** In this paper, we mainly focus on how the behavior of numerical schemes depends on the time-step size. For a given finite element mesh, we compare solutions of fully discrete schemes to those of semi-discrete schemes (namely, no discretization on time variables). It is possible that the solution of semi-discrete scheme is not a good approximation to the original phase-field model. We reach the following conclusions:

1. The first-order CSS is mathematically equivalent to a standard FIS with a (much) smaller time-step size. As a result, a CSS would usually lead to approximation of the solution of the original model at a delayed time. For the Allen-Cahn model, we have easily proved this time-delay effect rigorously. For the Cahn-Hilliard model, we observe that, from the numerical experiments, CSS also has a similar time-delay effect for the Cahn-Hilliard model. This seems to indicate that the solution of the regularized model (2.25) will probably have a time-delay effect in comparison to the solution of the original Cahn-Hilliard model (1.2).

2. Since CSS is really an FIS scheme (at least for the cases we have studied in this paper), we should not underestimate the value of other FIS. Thus we proposed a modified FIS so that the maximum principle holds on the discrete level and, as a result, a Poisson-like preconditioner can be devised and rigorously analyzed.
3. The advantage of any partially implicit scheme is to allow large time-step size. But these schemes with large time-step size would have serious time delay. This means the advantage is no longer clear for any partially implicit schemes, see Figure 4.1b.
4. Most schemes are convex when  $k$  is sufficiently small, which often leads to the energy-stability. Now that a fully implicit scheme becomes convex when  $k$  is sufficiently small, there is no-need to use any partially implicit scheme in this case.
5. *In summary*, we recommend to use FIS or (modified) Crank-Nicolson scheme by choosing  $k$  to be “convexity size” (with locally refined finite element grids). In this case, the Jacobi matrix is SPD and can be effectively preconditioned.

While most partially implicit schemes have been developed as a numerical technique for solving a given phase-field model, given the insight obtained in this paper, we would like to argue that it may be helpful to view the convex splitting technique as a discrete modeling technique, namely a procedure to convexify the original model. The convexified models are (2.30) and (2.31) for the Allen-Cahn Model and the Cahn-Hilliard equation, respectively. While neither (2.30) nor (2.31) has a corresponding convexity property on the continuous level, their appropriately discretized model would have the desired “uniform convexity” properties as stated in Theorem 2.8.

Partially implicit schemes (especially CSS) have been used for many different models that are different from or more complicated than both the Allen-Cahn and Cahn-Hilliard equations. We have not studied carefully how these schemes behave in those models, but hopefully our findings in this paper on partially implicit schemes for both the Allen-Cahn and Cahn-Hilliard models will give some new insight into the nature of convex splitting technique.

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